



chain nodes :

10 11 16 21 22 23 24 25 26 29 30 31 32 45

ring nodes :

1 2 3 4 5 6 12 13 14 15 35 36 37 38 39 40 41 42 43 44

chain bonds :

2-10 5-21 10-11 11-12 14-16 21-22 21-23 23-24 24-25 24-29 25-26 29-30 30-31 31-32
31-35 37-45

ring bonds :

1-2 1-6 2-3 3-4 4-5 5-6 12-13 12-14 13-15 14-15 35-36 35-40 36-37 37-38 38-39
38-41 39-40 39-44 41-42 42-43 43-44

exact/norm bonds :

1-2 1-6 2-3 2-10 3-4 4-5 5-6 5-21 10-11 11-12 12-13 12-14 13-15 14-16 14-15
21-22 21-23 23-24 24-25 24-29 25-26 29-30 30-31 31-32 31-35 35-36 35-40 36-37
37-38 37-45 39-40

normalized bonds :

38-39 38-41 39-44 41-42 42-43 43-44

G1:C,N

G2:O,N

Match level :

1:Atom 2:Atom 3:Atom 4:Atom 5:Atom 6:Atom 10:Atom 11:CLASS 12:Atom 13:Atom 14:Atom
15:Atom 16:CLASS 21:CLASS 22:CLASS 23:CLASS 24:CLASS 25:CLASS 26:Atom 29:CLASS
30:CLASS 31:CLASS 32:CLASS 35:Atom 36:Atom 37:Atom 38:Atom 39:Atom 40:Atom 41:Atom
42:Atom 43:Atom 44:Atom 45:CLASS

Generic attributes :

10:
Saturation : Unsaturated
Number of Carbon Atoms : less than 7
Type of Ring System : Monocyclic
26:
Saturation : Unsaturated

